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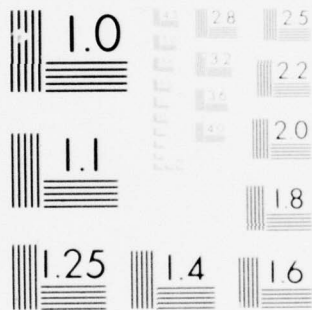
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Experimental and Theoretical Study of the
Electronic Properties of CdSiP_2 , CdSnP_2 ,
 CdSiAs_2 and CdSnAs_2

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by

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This report concerns the accomplishments made during the period of June 1, 1976 to June 30, 1977. The results will be divided into three different categories: I. The chalcopyrites, II. The ternary semiconductors, and III. The transition metals.

I. The Chalcopyrites.

A. Optical Properties:

1. Reflectance system:

We have made significant improvements on the optical reflectance system. These improvements were essentially due to the full utilization of a microcomputer, which is now being used to control experiments and process measured data. The computer incorporates a feedback loop through which the incident signal is maintained at a constant value at all wavelengths. Consequently, the reflectivity is always directly proportional to the reflected signal. Moreover, because high accuracy in the incident signal is thereby achieved (convergence to a fixed value of the incident signal involves an error of less than 0.1%), high accuracy in the reflectivity spectra is thus assured. Such high accuracy in measuring the reflectance spectra of the present crystals was critically needed because their small sizes resulted in low reflectance intensities. The development of this system required the design and construction of digital to analog and analog to digital interfacing, as well as all the software necessary to control the experiments.

2. Optical measurements:

Reflectance measurements were completed on the CdSnAs_2 , CdSnP_2 , and CdSiP_2 crystals (Figs. 1 - 3). The measured spectra

of the first two crystals show good agreement with the previous measurements of Stokowski.² Furthermore, the CdSnAs_2 spectrum agrees fairly well with its theoretically derived counterpart.

The reflectance spectrum of the CdSiP_2 crystal exhibits the same features of a large low-energy peak observed in the other chalcopyrite crystals; however, this peak is shifted to higher energy (3. eV).

B. Theoretical Studies:

The band structure of CdSnAs_2 along the Σ symmetry direction is shown in Fig. 4. The fundamental gap is direct, with a value of 0.65 eV. Experimental data on the gap for CdSnAs_2 is unavailable, but the present value is comparable to that obtained by Shileika¹ (0.5 eV) for CdGeAs_2 . The arrow in Fig. 4 indicates the location ($\vec{k} = (.167 .167 .0)2\pi/c$) of a second minimum in the lowest conduction band. Such a feature suggests the CdSnAs_2 may exhibit the Gunn effect. The calculated reflectivity, which is based on the above band structure, is compared in Fig. 5 to the experimental data. There is a general agreement between the spectra, with a one-to-one correspondence of all important structures. The locations of these structures agree to within 0.2 eV, suggesting that the present band structure is also accurate to within 0.2 eV.

II. The Ternary Semiconductors.

A. Crystal Growth:

Using the crystal growing system we developed, we were able to grow crystals of SbSeI and SbSBr larger than those grown previously. Crystal sizes were sufficiently large to

provide adequate reflectance for optical measurements and to eliminate prismatic and multiple reflection effects in the region around the energy gap that had been observed earlier with smaller crystals.³ Photographs of the crystals are shown in Fig. 6.

B. Optical Measurements:

Reflectance measurements were completed on the SbSBr (Fig. 7) and SbSeI (Fig. 7). Each measured spectra shows three structures. These results have been used as inputs for the theoretical computation of the electronic band structure.

C. Theoretical Studies:

1. Improvements on earlier calculations of SbSI:

In the earlier calculations of SbSI by Fong et. al.³ the shape of the reflectivities with polarization parallel ($\vec{E} // \hat{C}$) and perpendicular ($\vec{E} \perp \hat{C}$) to the shortest axis of the crystal show significant disagreement with the experimental data, especially for $\hbar\omega > 3.2$ eV. Using the techniques developed for the transition metals and their compounds⁴ we are able to improve the earlier results. The present results give a fundamental indirect gap $\Gamma_6 \rightarrow S_1$ at 2.11 eV which is in excellent agreement to the values of 2.05 and 2.20 eV for the two polarizations observed in Raman spectroscopy.⁵ As shown in Fig. 7, the shapes of the theoretical and experimental reflectivities agree reasonably well. The calculated positions of the structures in the reflectivities differ by no more than 0.2 eV from the corresponding measured values. The band structure of SbSI is shown in Fig. 8. There are two minima: one along ΓX

and one along ΓZ . The results are consistent with the observed Gunn effect in SbSI by Sawaguchi and Mori.⁶

2. Band structures of SbSeI and SbSBr:

The measured optical data discussed in B. are used to determine the pseudopotentials of the constituents in these two compounds. The calculated band structures of the two crystals are shown in Fig. 8. The fundamental gaps of SbSBr and SbSeI are 2.18 and 1.67 eV respectively, which are in good agreement with the measured values of 2.22 (SbSBr) and 1.71 (SbSeI) eV.⁷ The derived reflectivities for the two compounds agree with measured ones to the order of 0.2 eV (Fig. 7).

The calculated band structures of SbSBr explicitly show two minima as in the case of SbSI, whereas only one minimum away from the symmetry points (Γ , X, Y, Z, S) is found in SbSeI. While we expect that both compounds should exhibit the Gunn effect, our results suggest that one could more readily detect the effect in SbSBr.

III. The Transition Metals:

We have studied the group V transition metals in depth by calculating the band structures, Fermi surfaces, charge densities, and the density of states. By comparing to experimental data such as reflectivities, Fermi surfaces, and X-ray data, the overall agreement between the theory and the experiment is better than 0.5 eV. We have also found that there is significant d - p

hybridization in these metals. This is in disagreement with the results of the argument-plane-wave method (APW). However, we believe the reason is due to the neglecting of the p-states in constructing the muffin-tin potential in the APW method.

Manuscript has been accepted for publication by Physical Review.

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Figure Captions

- Fig. 1 Reflectivity spectrum of CdSnAs_2 .
- Fig. 2 Reflectivity spectrum of CdSnP_2 .
- Fig. 3 Reflectivity spectrum of CdSiP_2 .
- Fig. 4 Band structure of CdSnAs_2 .
- Fig. 5 Comparison of theoretical and measured reflectivities of CdSnAs_2 .
- Fig. 6 Photographs of ternary compounds - crystals of SbSBr and SbSeI .
- Fig. 7 Reflectivity spectra of SbSI , SbSBr and SbSeI .
- Fig. 8 Band structures of SbSBr , SbSI and SbSeI .

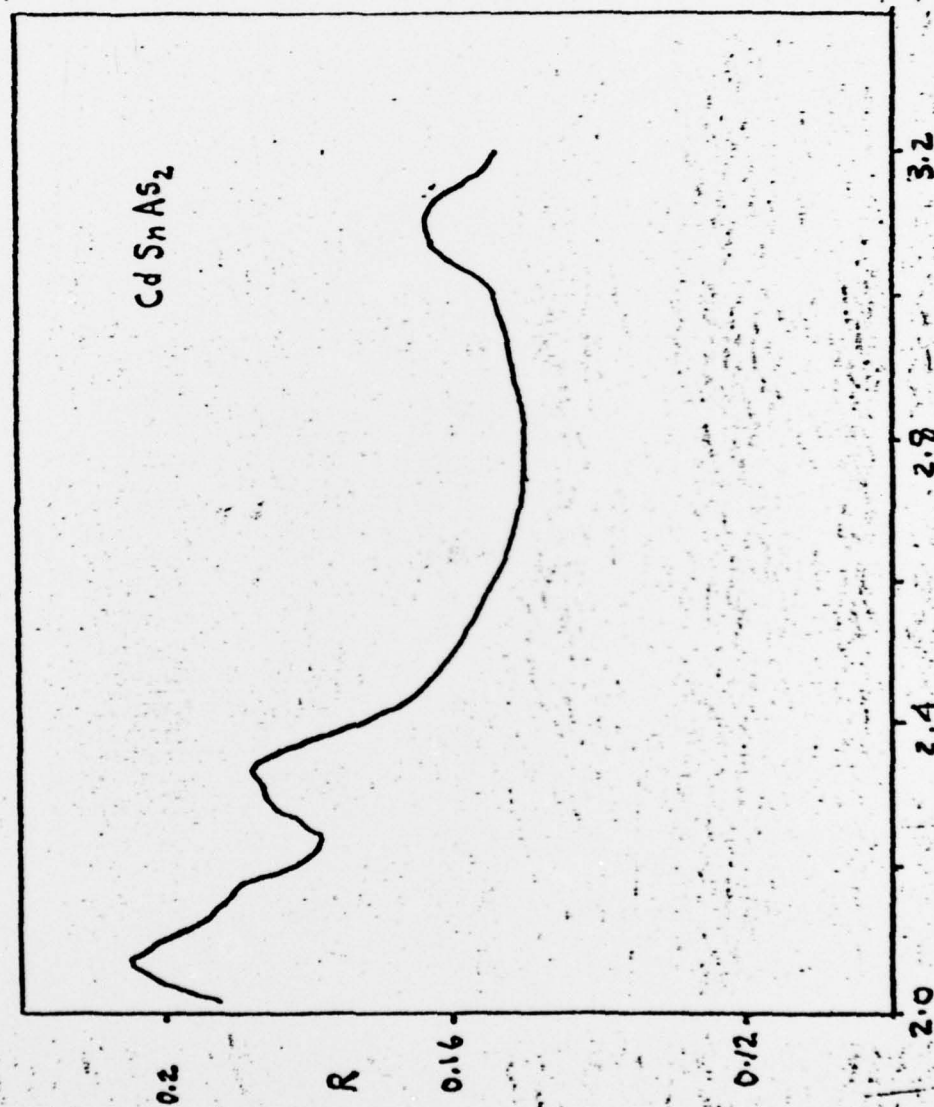


Fig 1

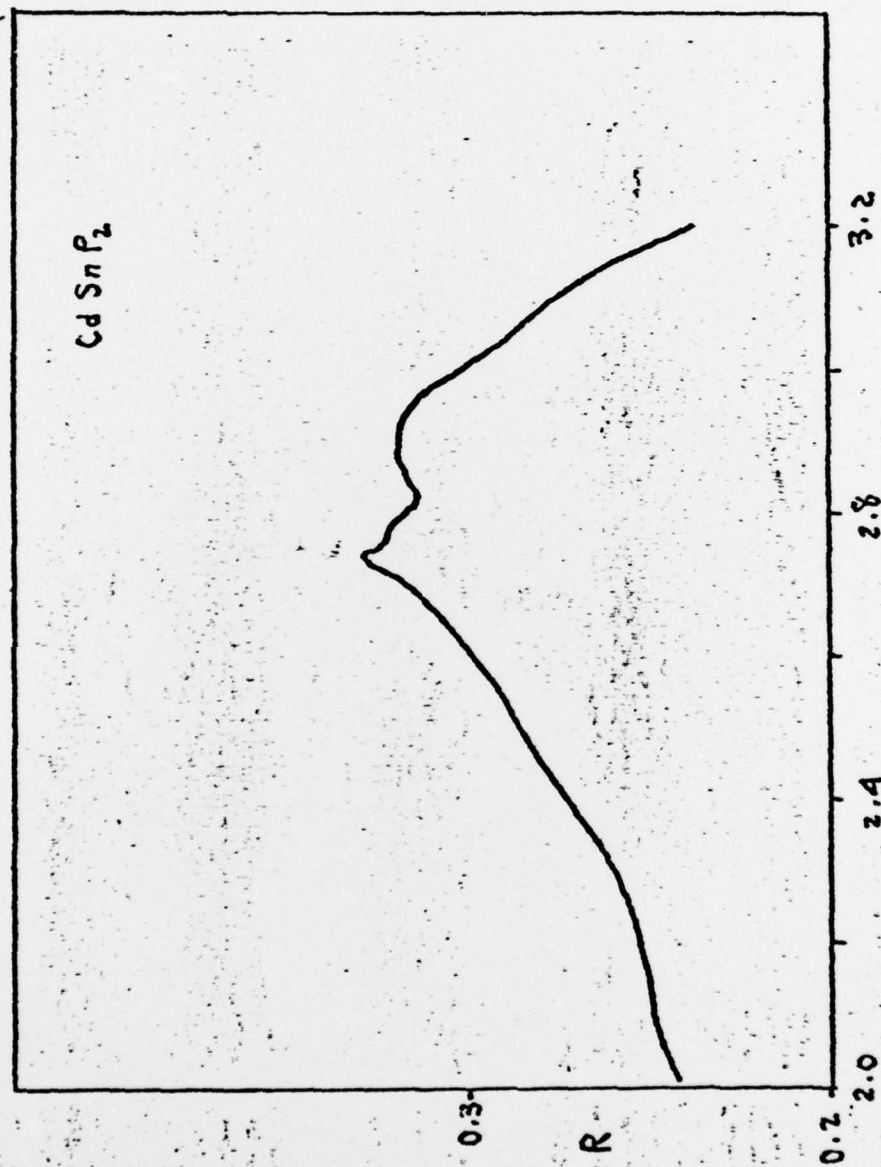


Fig 2

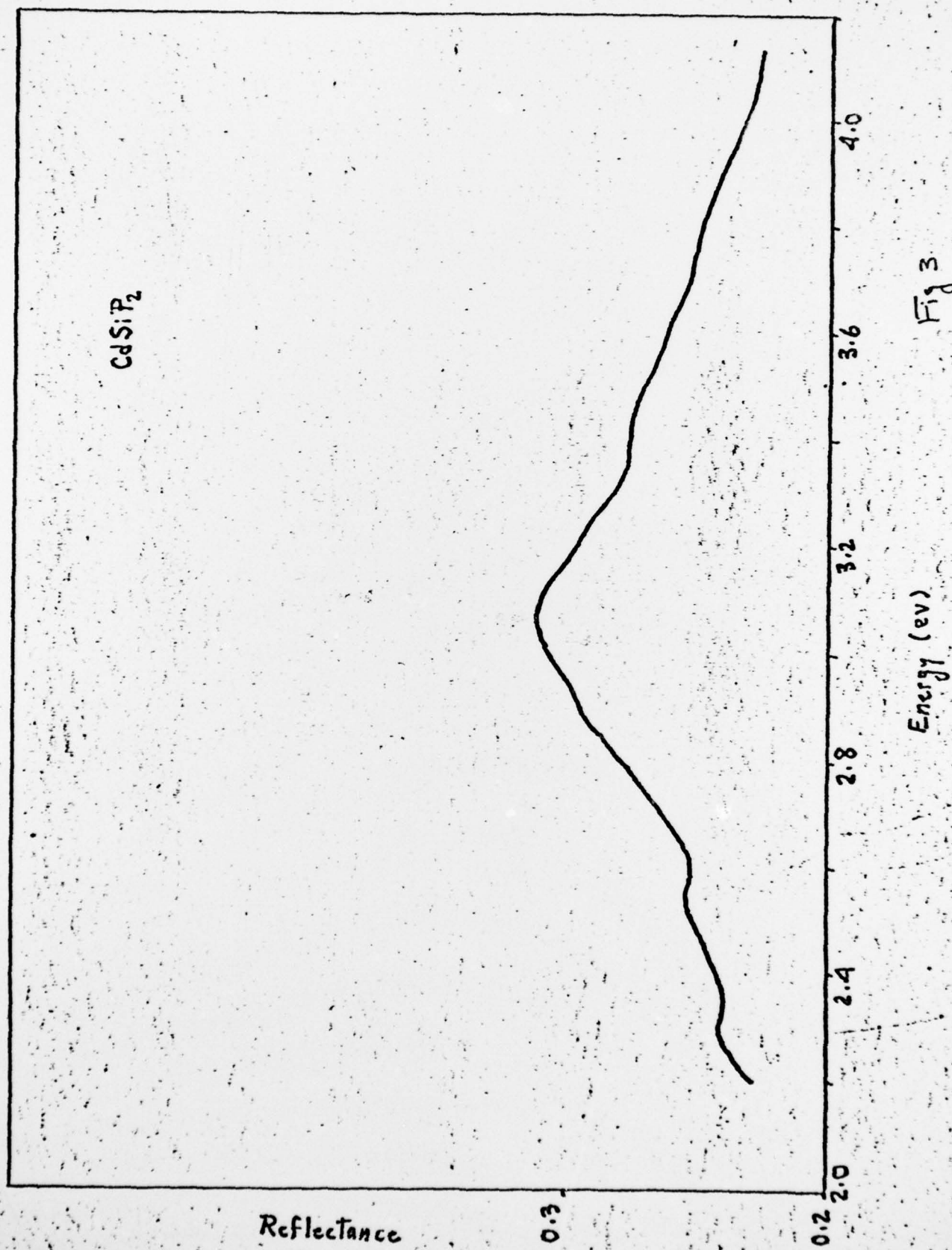


Fig 3

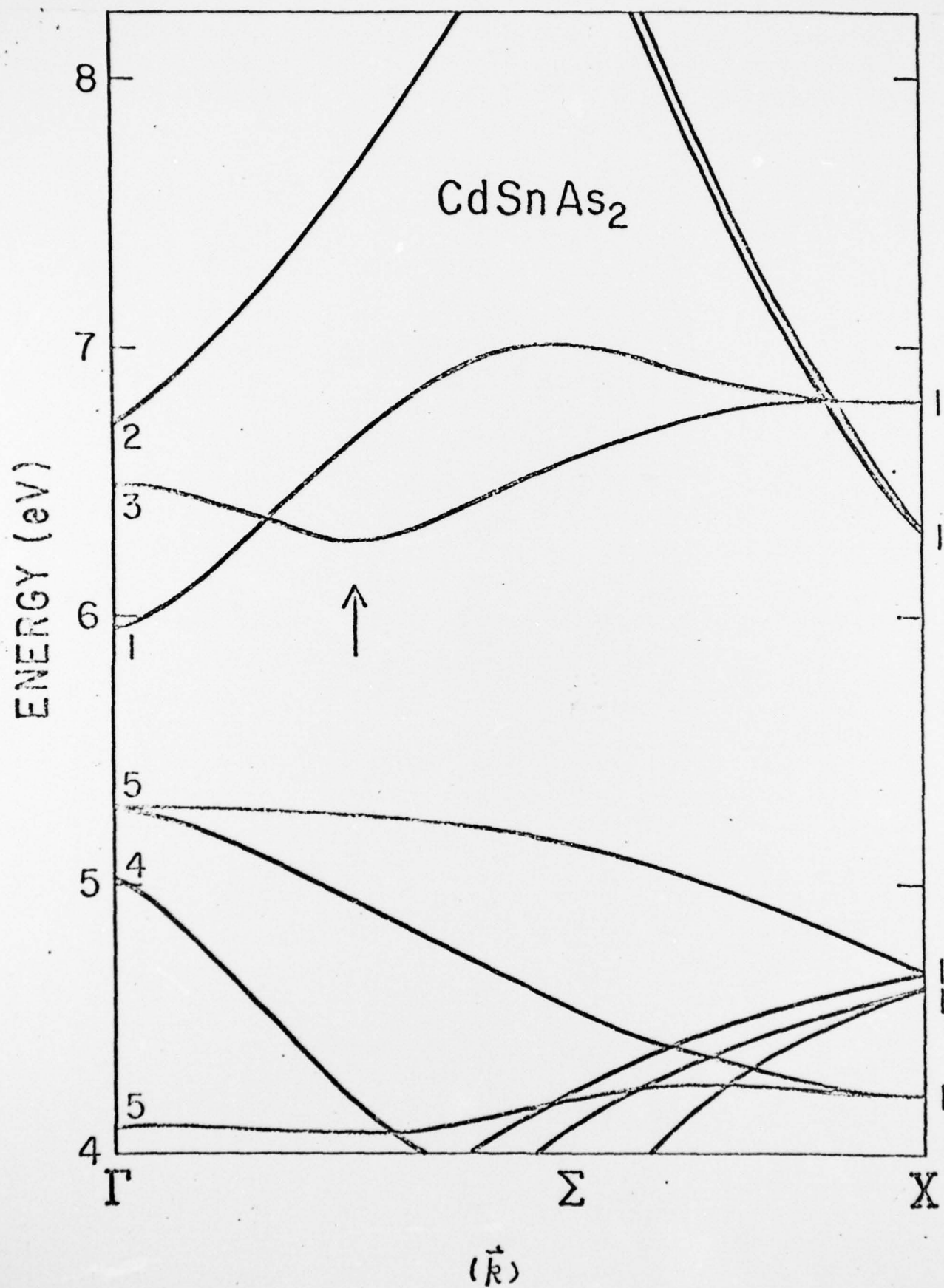


Fig. 14

CdSnAs_2

REFLECTIVITY

0.20

0.10

— THEORY

- - - DATA

2

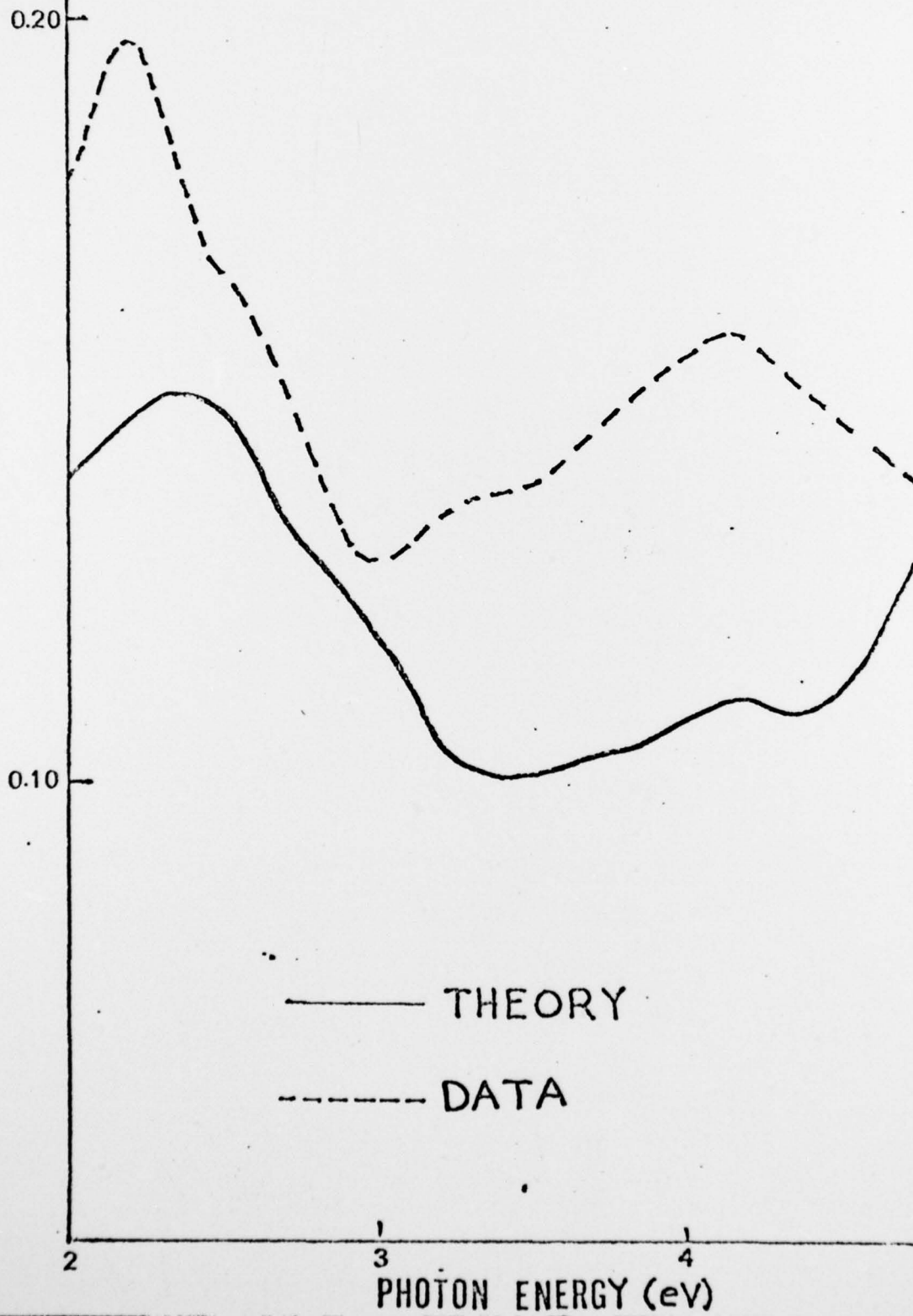
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PHOTON ENERGY (eV)

Fig. 5



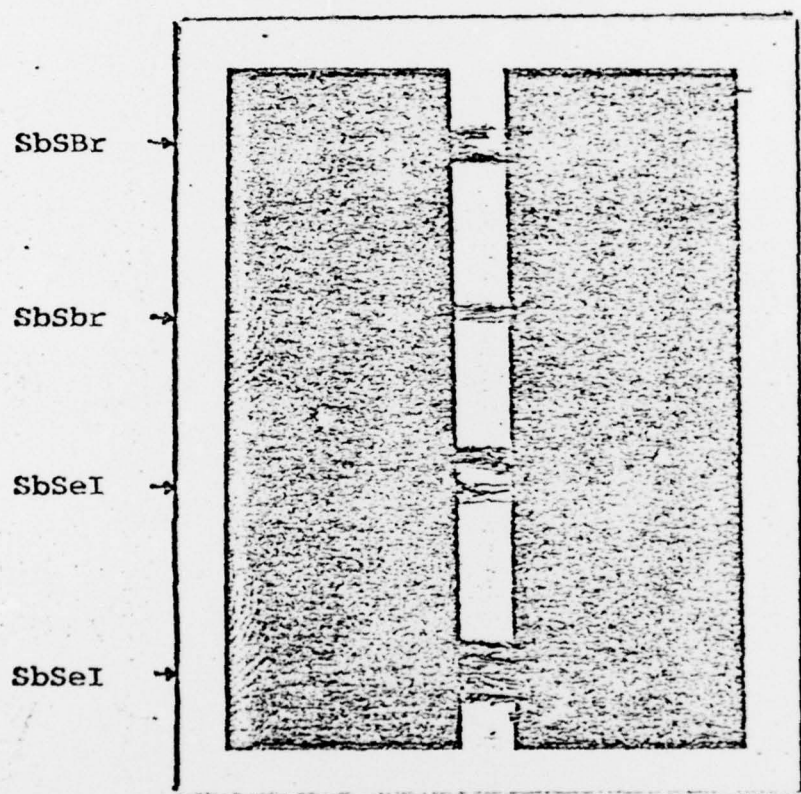


Fig. 6

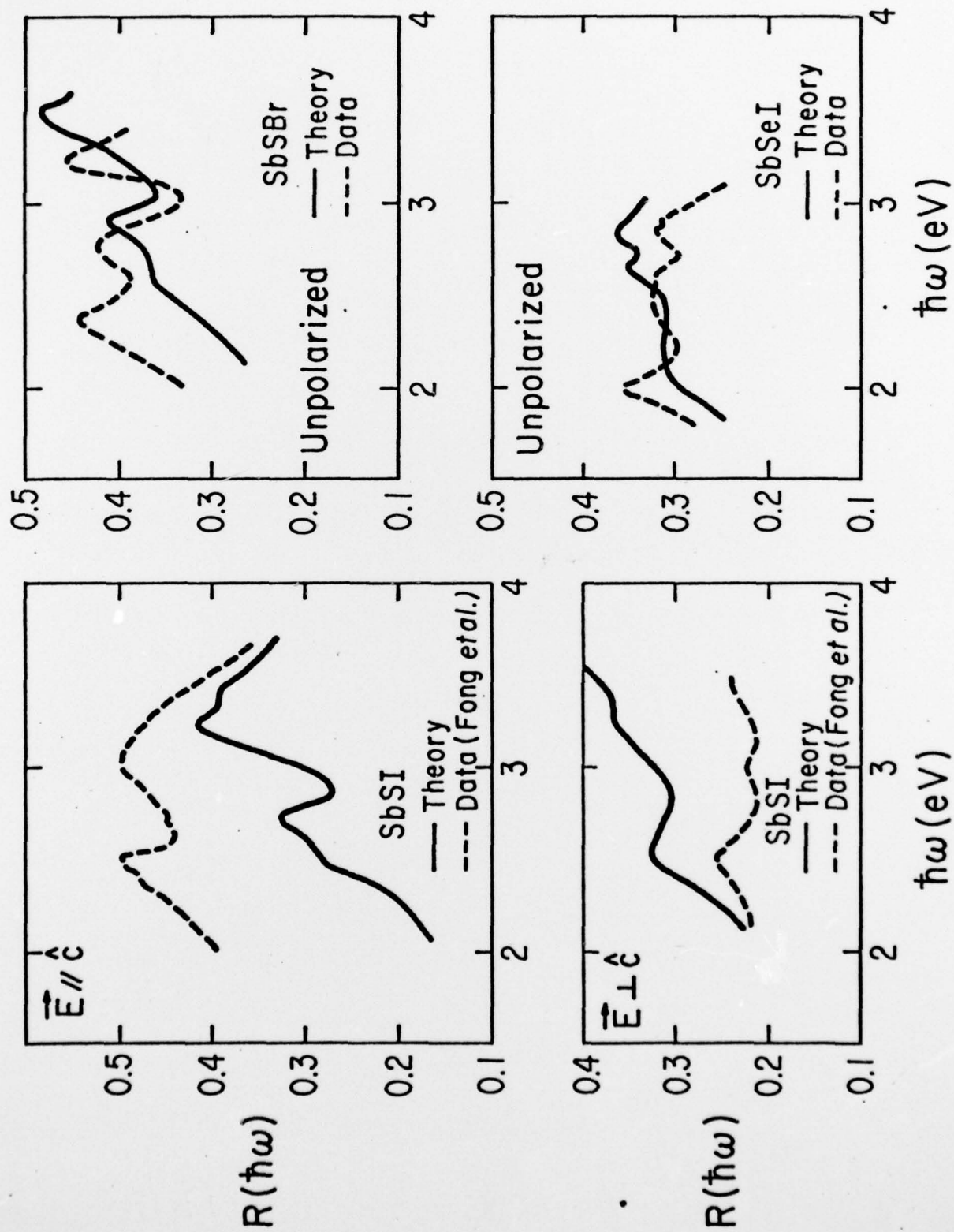


Fig. 7

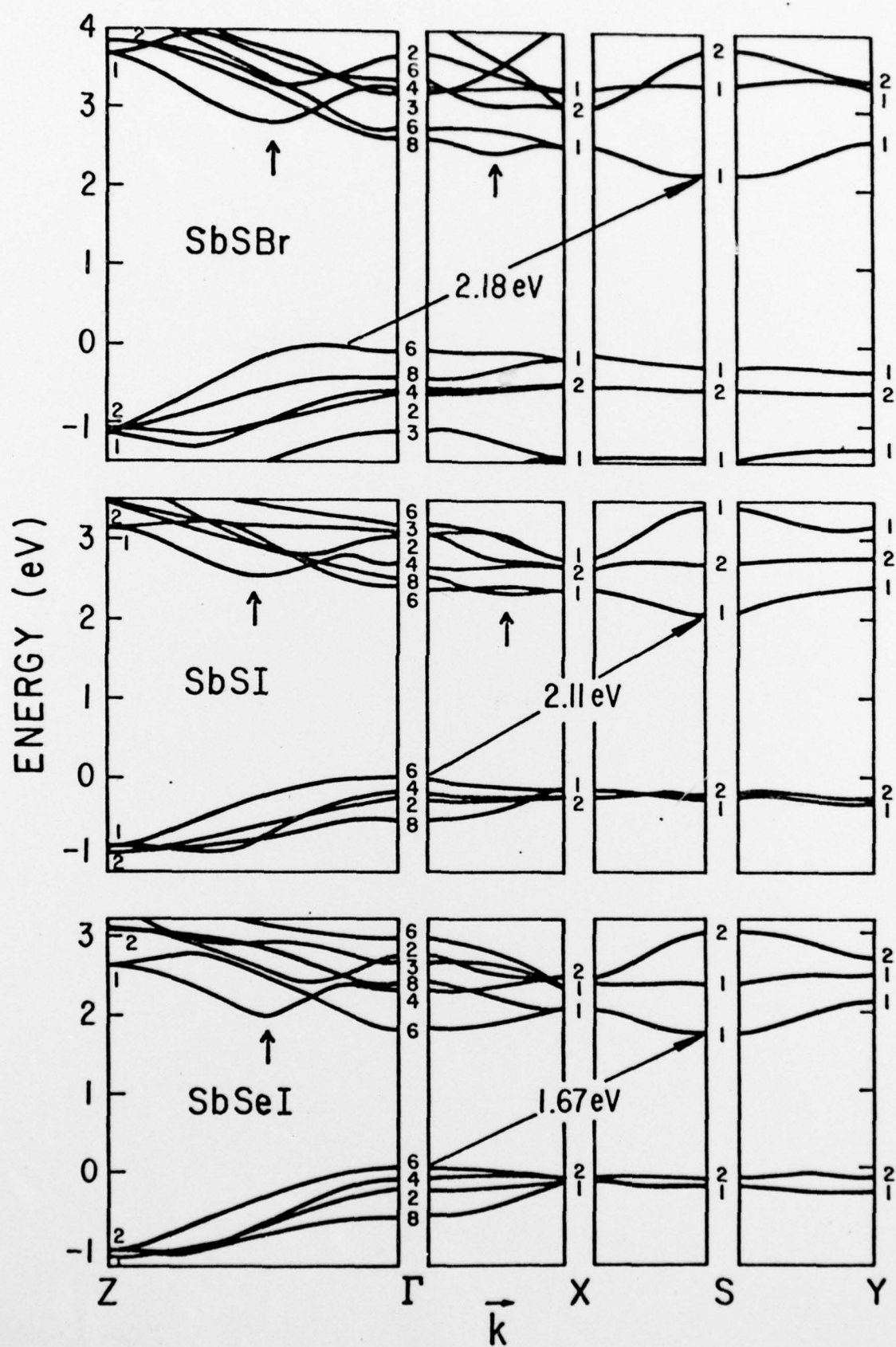


Fig. 8

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Optical reflectivities of CdSnAs_2 , CdSiP_2 , CdSnP_2 , SbSBr and SbSeI have been measured. Results of CdSnAs_2 , SbSBr, SbSeI are compared with theoretical calculations using the empirical pseudopotential method. Improved theoretical results of SbSI are also presented. Other contributions of transition metals are included.		